Finite Element Modeling Of Multiwalled Carbon Nanotube

A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS

FOR THE DEGREE OF

Bachelor of Technology in Mechanical Engineering

Thesis Submitted By

Rakesh Prabu.T
Roll No: 10603034

Guided By

Prof. Tarapada Roy

DEPARTMENT OF MECHANICAL ENGINEERING

NATIONAL INSTITUTE OF TECHNOLOGY ROURKELA

Orissa-769008, India.

May, 2010

CERTIFICATE

This is to certify that the thesis entitled "***Finite Element Modeling of Multiwalled Carbon Nanotubes*"** submitted by **Rakesh Prabu T (Roll Number: 10603034)** in partial fulfillment of the requirements for the award of ***Bachelor of Technology*** in the department of Mechanical Engineering, National Institute of Technology, Rourkela is an authentic work carried out under my supervision and guidance.

To the best of my knowledge, the matter embodied in the thesis has not been submitted to elsewhere for the award of any degree.

Place: Rourkela
Date: 13,May,2010

Prof. Tarapada Roy
Mechanical Engineering Department
National Institute of Technology
Rourkela-769008

ACKNOWLEDGEMENT

It gives me immense pleasure to express my deep sense of gratitude to my supervisor **Prof. Tarapada Roy** for his invaluable guidance, motivation, constant inspiration and above all his ever co-operating attitude enabled me in bringing up this thesis in present elegant form.

I am extremely thankful to **Prof. R. K. Sahoo**, Head, Department of Mechanical Engineering and the faculty member of Mechanical Engineering Department for providing all kinds of possible help and advice during the course of this work.

It is a great pleasure for me to acknowledge and express my gratitude to my parents for their understanding, unstinted support and endless encouragement during my study.

I am greatly thankful to all the staff members of the department and all my well wishers, class mates and friends for their inspiration and help.

Lastly I sincerely thank to all those who have directly or indirectly helped for the work reported herein.

Rakesh Prabu.T
(Roll Number: 10603034)
Department of Mechanical Engineering
National Institute of Technology, Rourkela

Contents

ABSTRACT

Three-dimensional finite element (FE) model for armchair, zigzag and chiral single-walled carbon nanotubes (SWCNTs) is proposed. The model development is based on the assumption that carbon nanotubes, when subjected to loading, behave like space-frame structures. The bonds between carbon atoms are considered as connecting load-carrying members, while the carbon atoms as joints of the members.To create the FE models, nodes are placed at the locations of carbon atoms and the bonds between them are modeled using three-dimensional elastic beam elements. The elastic moduli of beam elements are determined by using a linkage between molecular and continuum mechanics. The investigation includes armchair and zigzag SWCNTs.

It is found that the choice of Vanderwall forces, the interaction significantly affects the calculation of Young's modulus. The obtained values of Young's modulus agree very well with the corresponding theoretical results and many experimental measurements. Dependence of elastic moduli to diameter and length of the nanotubes is also obtained. The presented results demonstrate that the proposed FE model may provide a valuable tool for studying the mechanical behavior of carbon nanotubes and their integration in nanocomposites.
So for we dealt with single walled carbon nanotube, in our case, we are going to consider into doubled walled carbon nanotube generally speaking multi-walled carbon nanotube. The therefore properties so obtained is completely different that of single walled. The DWCNT is then modeled in ANSYS-multiphysics then in is analysed for the mechanical properties using the same. The elements were considered as beam4, it is an uniaxial element with tension, compression, torsion, and bending capabilities. The element has six degrees of freedom at each node: translations in the nodal x, y, and z directions and rotations about the nodal x, y, and z axes. Stress stiffening and large deflection capabilities are included.
The interaction between the two layers of the MWCNT, the Vanderwalls interation, is considered in the calculation of mechanical parameter .The interation are also made of beam4 element, which researchers have not so far attempted to work on.

2. Introduction:

2.1 Composites and Nano-composites:

Composite materials are engineered material made from two or more constituent materials with significantly different physical or chemical properties which remain separate and distinct on a macroscopic level within the finished structure.

Where as a **nanocomposite** is as a multiphase solid material where one of the phases has one, two or three dimensions or structures having nano-scale repeat distances between the different phases that make up the material. The definition can include porous media, colloids, gels and copolymers, but is more usually taken to mean the solid combination of a bulk matrix and nano-dimensional phase differing in properties due to dissimilarities in structure and chemistry

Nanocomposites differ from conventional composite material due to the exceptionally high surface to volume ration of the reinforced phase or its exceptionally high aspect ratio. Say large amount of reinforcement surface means that a relatively small amount of nanoscale reinforcement can have an observable effect on the nanoscale properties of the composites. For example adding carbon nanotubes improves the electrical and thermal conductivity, it also increases optical and dielectric ,heat resistance , mechanical properties like stiffness, strength, resistance to wear and damage.

2.2 Carbon Nanotubes:

Carbon nanotubes are hollow cylinders with diamneters ranging from 1 nm to 50 nm and length over 10 μm. They consist of only carbon atoms and can be thought of as a graphite sheet that has been rolled into a seamless cylinder.

There are two kinds of nanotubes; One is a single-wall nanotube that is made up of a single layer of graphite ("graphene" sheet) and the other is a multiwall nanotube that consists of multiple shells.

Nanotubes have aroused great interest recently because of their unique physical properties, which span a wide range from structural to electronic. For example, nanotubes have a light weight and high elastic modulus, and thus they are predicted to the strongest fibers that can be made. Their high strength is accompanied by their ability to buckle in a reversible manner.

When the nanotube is bent, it does not fracture but buckles like a rubber hose. Then, carbon nanotubes, especially SWNTs, possess the exceptional electronic properties; they can be metallic or semimetallic, depending on the geometry how a graphene sheet is rolled up into a tube. The carbon nanotube especially single walled nanotube posses the exceptionally single called nanotubes posses exceptional electronics properties , they can be metallic and semi metallic depending on geomentrical properties, carbon nanotubes exhibits high stiffness, strength and resilience.

As a consequence, they may provide the ideal reinforcing material for a new class of nano-composite. Although carbon nanotubes can be used as conventional carbon fiber to reinforce polymer matrix in order to form advanced nano-composites, they may be also used to improve the out of plane and inter laminar properties of current advanced composite materials.

The potential use of carbon nanotube as reinforcing material in nano-composite has originated the need to explore their exact mechanical loading and as a subsequent step, identify the possible failure mechanism that may appear.

The characteristics of carbon nanotube are more complex than that of conventional material due to dependence of their mechanical properties on size and nano structure.

3.Literature Review:

Since the discovery of carbon nanotube by Iijima[1] , researchers put their utmost efforts to find its property of the same. Carbon nanotubes show finds a wide range of applications in physics and engineering. However, understanding the CNT is still a mystery because of its nanosize which prevents from physical experiments. Researchers tried to find the properties of single walled and multiwalled carbon nanotube properties, this lead to many theories regarding carbon nanotubes and followed by the many results regarding the same parameter.

Few even tried experimental investigations,it was found that modulus of MWNTs has mean value of 1.8 TPa with a variation from 0.40 to 4.15 TPa[2] , Krishnam et al[3] also used TEM and observed the vibration of SWNT and obtained the Young's modulus ranged from 0.90 to 1.70 TPa, Wang et al.[4] conducted bending tests on cantilevered tubes using atomic force microscopy and calculated the modulus to be of 1.28 TPa. Poncharal et al.[5] observed the static and dynamic mechanical deflections of cantilevered MWNTs and a modulus of about 1.0 TPa is obtained.

Our approach is by continuum finite element method which was conducted by Zhang et al.[6][7] Jin and Yuan Li and Chou.[8][9] Here a nanotube can be well described as a continuum solid beam tension, bending, or torsional forces, it is reasonable to model the nanotube as a frame or shell-like structure, then the mechanical properties of such a structure can be obtained by classical continuum mechanics or finite element method. Thanks to the uncertainty of the CNT wall thickness Which again lead to many theories and in turn paved for many results, ranged from about 1.0 to 5.5 TPa a modulus value can be found from the researchers work. We have developed a finite element model of SWNTs and consequently estimated their mechanical property namely Young's modulus. [10]

As explained earlier the concept is that concept the carbon nanotube can be treated as a framelike structure, and the interaction between the atoms which has the bond length as a beam element. Tserpes and Papanikos[11] have calculated the moduls on the same fashion as above, they used ANSYS code for the generation of the model and more efficient calculation of all the parameters on the frame structure.

Efforts were made easy in SWCNT but in advent of MWCNT's, the interaction between the layers due to vander waal forces comes into picture, it should to taken care that only for a finite distance this effect is felt, to Li and Chou[8] used truss elements to simulate the interlayer vander Waals force of MWNTs.

In our case its going to be the beam element, the same type of element used for covalent bond interaction in the layers of MWCNTs. As it was said Vanderwall forces are considered to be weaker than covalent, in order to cope with this effect the number of interactions between the neighboring atoms are reduced and there by the interaction forces are turned to beam type and the modulus was calculated and further similar types of simulation/analysis are carried on.

4. Atomic Structure of Carbon Nanotube(CNT):

There are two types of CNTs: Single walled carbon nanotube(SWCNT) and multiwall carbon nanotube(MWCNT). MWCNTs are composed of co-axially situated SWCNTs of different radii. There are several ways to view a SWCNT. The most widely used is by reference to rolling up grapheme sheet to form a hollow cylinder with end caps.

The cylinder is composed of hexagonal carbon rings[12], while the end caps of pentagonal rings. The hexagonal pattern is repeated periodically leading to binding of each carbon atom to three neighboring atoms with covalent bonds. This covalent bond is a very strong chemical bond and plays significant role to the impressive mechanical properties of graphitic and as a consequence, of all carbon-related nano-structures. The atomic structure of nanotubes depends on tube chirality, which is defined by the chiral vector C_h and the chiral angle θ. The chiral vector is defined as the line connected from two crystallographically equivalently sites O and C on a two-dimensional graphene structure. The chiral vector C_h can be defined in terms of the lattice translation indices (n, m) and the basic vectors a_1 and a_2 of the hexagonal lattice as follows $C_h = n\vec{a}_1 + m\vec{a}_2$ (1)

The chiral angle θ is the angle between the chiral vector C_h with respect to the zigzag direction (n, 0) where $\theta=0^0$ and the unit vectors a_1 and a_2. For the chiral angles of 0 and 30^0, the armchair and zigzag nanotubes are formed, respectively.

These two types of nanotubes correspond to the two limiting cases. In terms of the roll-up vector, the armchair nanotubes are defined by (n, n) and the zigzag nanotubes by (n, 0).
For chiral angles different than 0 and 30^o, the chiral nanotubes, which are defined by a pair of indices (n, m) where $n \neq m$ are formed. Schematic representations of the three types of nanotubes is shown in Fig. 1.

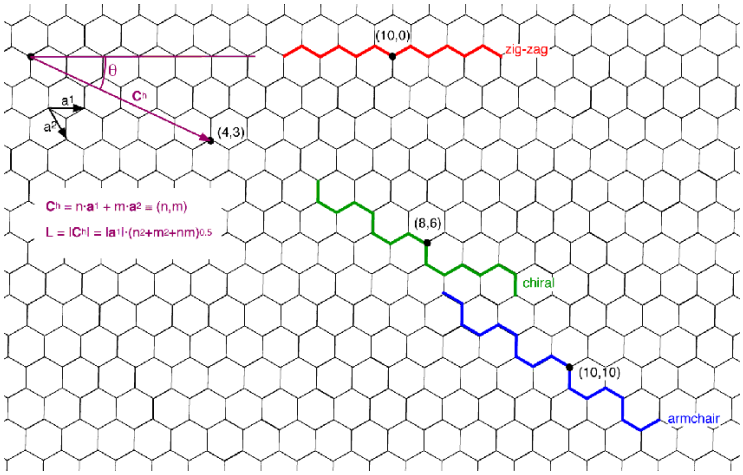


Fig. 1 Schematic of the hexagonal lattice of graphene sheet including definition of basic structural parameters. (http://ipn2.epfl.ch/CHBU/NTbasics1.htm)

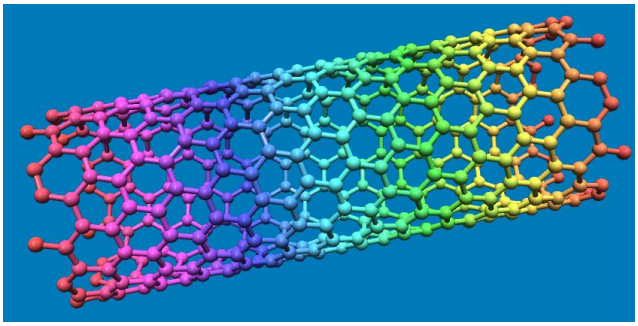


Fig. 2 a Schematic of armchair

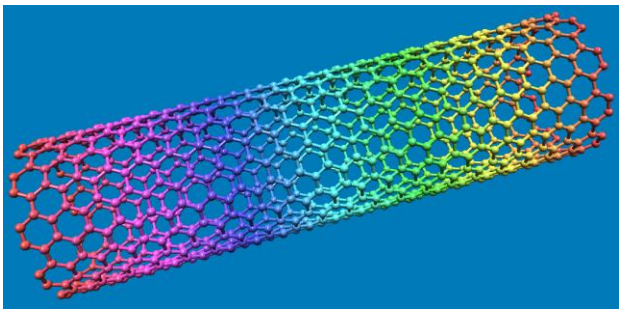


Fig. 2 b Schematic of ZigZac

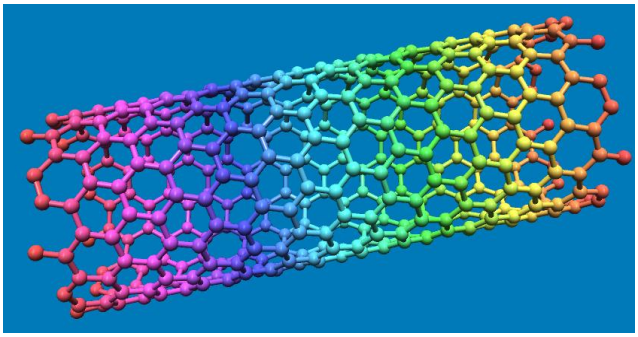
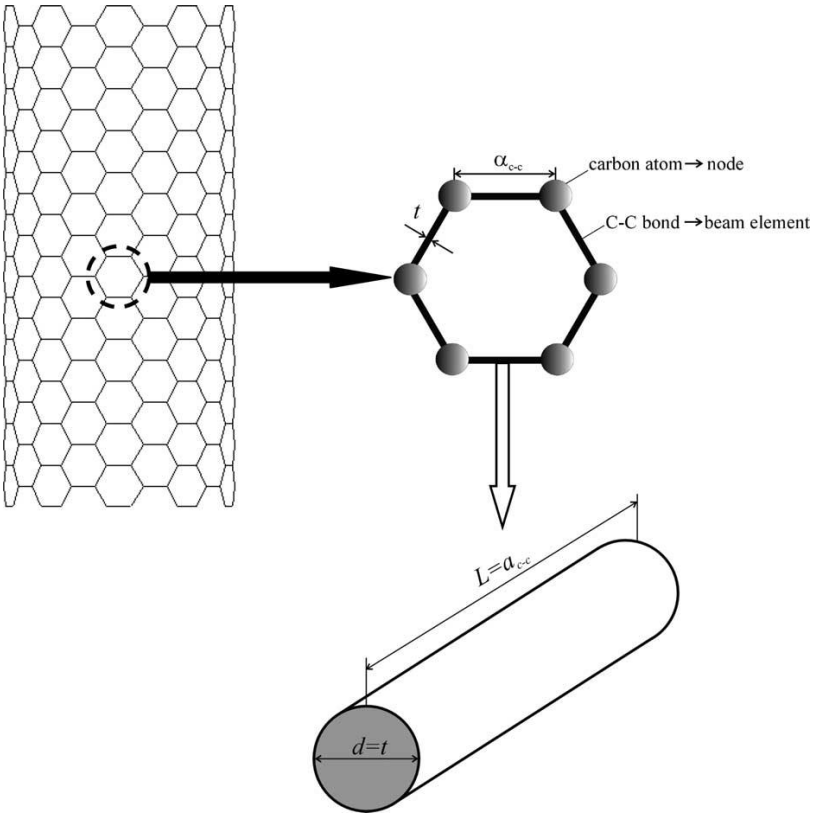


Fig. 2c Schematic of Chiral

5. Finite Element Modeling:

CNTs carbon atoms are bonded together with covalent bonds forming an hexagonal lattice. These bonds have a characteristic bond length a_{C-C} and bond angle in the 3D space. The displacement of individual atoms under an external force is constrained by the bonds. Therefore, the total deformation of the nanotube is the result of the interactions between the bonds. By considering the bonds as connecting load-carrying elements, and the atoms as joints of the connecting elements, CNTs may be simulated as space-frame structures.



By treating CNTs as space-frame structures, their mechanical behavior can be analyzed using classical structural mechanics methods. In this work, a 3D FE model able to assess the mechanical properties of SWCNTs is proposed.

The 3D FE model is developed using the ANSYS commercial FE code. For the modeling of the bonds, the 3D elastic BEAM4 ANSYS element is used. The specific element is a uni-axial element with tension, compression, torsion and bending capabilities.

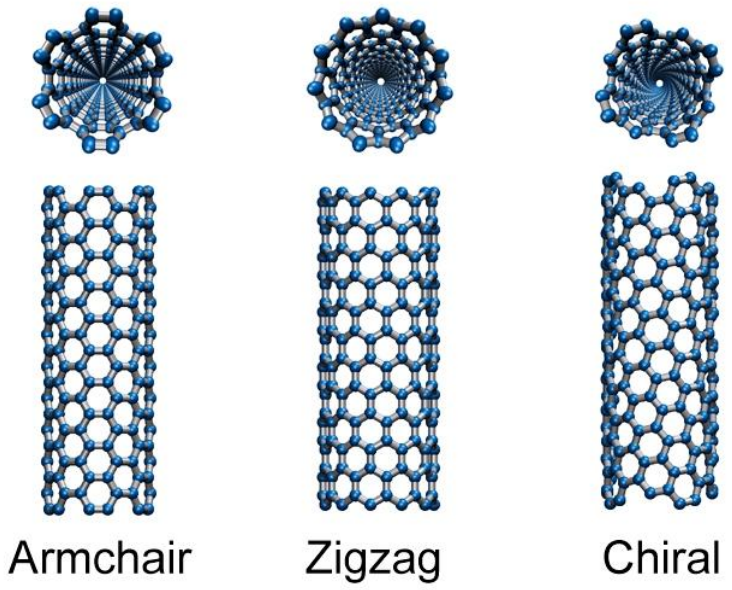


Fig.4 Front view and top view of the finite element mesh.

It has six degrees of freedom at each node: translations in the nodal x, y, and z directions and rotations about the nodal x, y, and z-axes. The element is defined by two or three nodes as well as its cross-sectional area, two moments of inertia, two dimensions and the material properties.

The 3D FE model is developed using the ANSYS commercial FE code. For the modeling of the bonds, the 3D elastic BEAM4 ANSYS element is used. The specific element is a uni-axial element with tension, compression, torsion and bending capabilities. It has six degrees of freedom at each node: translations in the nodal x, y, and z directions and rotations about the nodal x, y, and z-axes. The element is defined by two or three nodes as well as its cross-sectional area, two moments of inertia, two dimensions and the material properties.

The hexagon, which is the constitutional element of CNTs nano-structure, is simulated as structural element of a space-frame. In the same way the entire nanotube lattice is simulated. The simulation leads to the correspondence of the bond length a_{C-C} with the element length L as well as the wall thickness t with the element thickness. By assuming a circular cross-sectional area for the element, as in the previous page figure, t corresponds to the element diameter d.

Although CNTs are hollow cylinders with closed caps at both ends, they are modeled as narrow cylinders with open ends in order to simplify the analysis. For the automatic generation of the FE models, a routine was created using the ANSYS macro-language.

The routine requires as input the Cartesian coordinates of carbon atoms and the bond length at the state of equilibrium. The FE model uses the coordinates of the carbon atoms for creating the nodes and then appropriate connection of the nodes generates the beam elements.

Initially, one beam element per bond was used in order to compare with the stiffness matrix method. However, convergence tests showed that if more elements are used, the results do not vary significantly.

This is attributed to the fact that stretching is the major form of deformation of the beam element simulating the atomic bond. The size of the FE model varied from 210 elements for the zigzag (5,0) configuration to 1988 elements for the armchair (20,20) configuration.

6.Multiwalled Carbon nanotubes:

A carbon nanotube can be considered as a large molecule consisting of carbon atoms, forming a hexagonal mesh. It may also be regarded as a one atom thick sheet of graphite, rolled into a tube with high aspect ratio. Such a tube can be considered as a fundamental structural unit, known as single-walled carbon nanotube.

Using that fundamental structural unit, a multi-walled carbon nanotube can be formed. MWNTs are in fact concentrically nested SWNTs, with a distance between the layers or walls equal to 0.34 nm.

Each atom in a single layer has three nearest neighbouring atoms and they are bonded by covalent bonds, which have characteristic properties (bond length and bond angle). Atoms on different layers of MWNTs are not connected by covalent bonds and the only interaction between them is through vander Waals forces. Vander Waals forces are rather weak compared to covalent bonds.

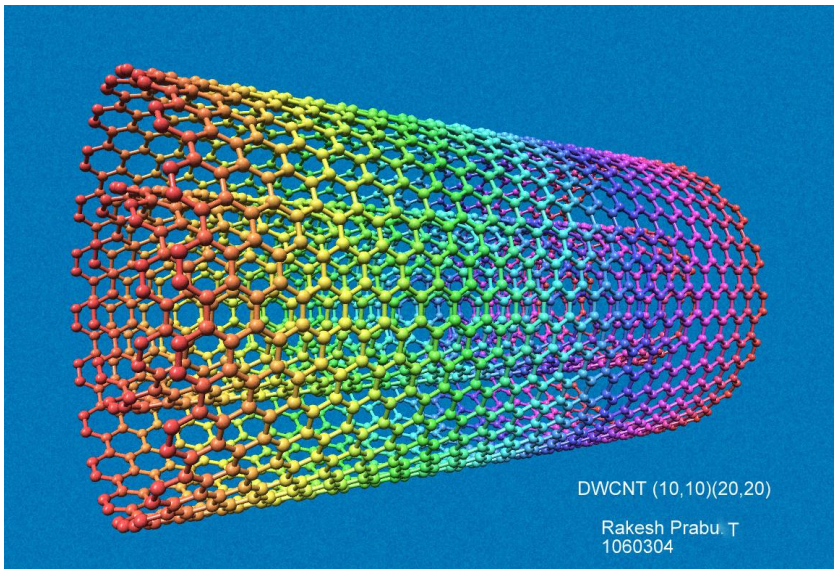


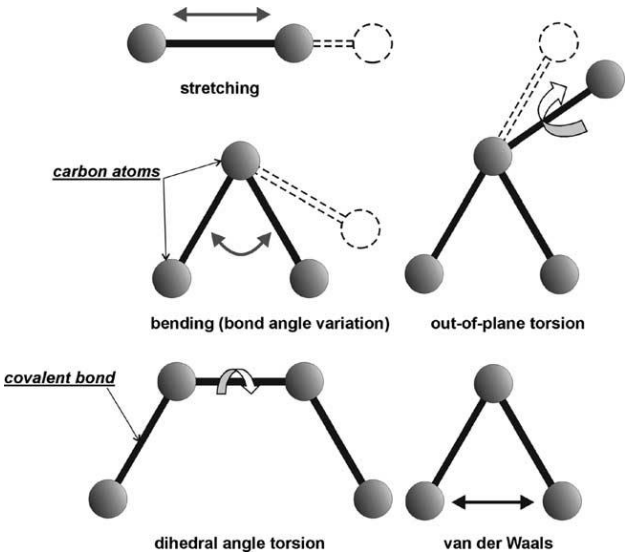
Fig. 5 Perspective view of DWCNT. The above figure is a double walled model, with close observation one can mark the presence of two layers. Especially the first layer covered by the second layer.

7. Formulation:

7.1 Elastic moduli of beam elements:

To calculate the elastic moduli of beam elements, a linkage between molecular and continuum mechanics is used.

From the viewpoint of molecular mechanics, CNTs may be regarded as large molecules consisting of carbon atoms. The atomic nuclei may be regarded as material points and their motions are regulated by a force-field generated by electron–nucleus and nucleus–nucleus interactions. The force-field is expressed in the form of steric potential energy, which depends solely on the relative positions of the nuclei constituting the molecule. The general expression of the total steric potential energy, when omitting the electrostatic interaction, is the following sum of energies due to valence of bonded interactions or bonded and non-bonded interactions[13].



←Fig. 6 Inter-atomic interactions in molecular mechanics.[11]

$$U_{total} = \sum U_r + \sum u_\theta + \sum u_\Phi + \sum u_w + \sum u_{vdw} \quad (2)$$

where U_r is the energy due to bond stretch interaction, U_θ the energy due to bending (bond angle variation), U_ϕ the energy due to dihedral angle torsion, U_ω the energy due to out-of-plane torsion and U_{vdw} the energy due to non-bonded Vander Waals interaction.

For covalent systems, the main contributions to the total steric energy comes from the first four terms of above equation Under the assumption of small deformation, the harmonic approximation is adequate for describing the energy[14]. By adopting the simplest harmonic forms and merging dihedral angle torsion and out-of plane torsion into a single equivalent term, we get for each energy.

$$u_r = \frac{1}{2}k_r(r - r_o)^2 = \frac{1}{2}k_r(\Delta \mathrm{r})^2 \qquad (3)$$

$$u_\theta = \frac{1}{2}k_\theta(\theta - \theta_o)^2 = \frac{1}{2}k_\theta(\Delta\theta)^2 \qquad (4)$$

$$u_\tau = u_\Phi + u_w = \frac{1}{2}k_\tau(\Delta\Phi)^2 \qquad (5)$$

where k_r, k_q, and k_t are the bond stretching, bond bending and torsional resistance force constants, respectively, while Δr, Δq and$\Delta\phi$ represent bond stretching increment, bond angle variation and angle variation of bond twisting, respectively. In order to determine the elastic moduli of beam elements, relations between the sectional stiffness parameters in structural mechanics and the force-field constants in molecular mechanics need to be obtained[4].

For simplicity reasons, the sections of the bonds are assumed to be identical and circular, and therefore the moments of inertia are equal, i.e. $I_x=I_y=I$. The elastic moduli that need to be determined are the Young's modulus E and shear modulus G. The deformation of a space-frame results in changes of strain energies.

Thus, the elastic moduli can be determined through the equivalence of the energies due to the interatomic interactions (Eqs. (3)–(5)) and the energies due to deformation of the structural elements of the spaceframe. As each of the energy terms of Eqs. (1)–(3) represents specific deformations, and no interactions are included, the strain energies of structural elements under specific deformations will be considered.

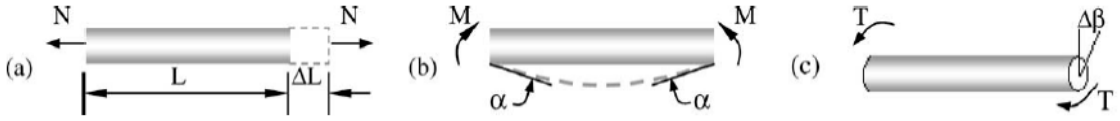


Fig. 5 Beam being stretched ,undergoing bending, torsion respectively[15]

According to classical structural mechanics, the strain energy of a uniform beam of length L and cross-section A under pure axial force N is

$$u_A = \frac{1}{2}\int_0^L \frac{N^2}{EA}dL = \frac{1}{2}\frac{N^2}{EA} = \frac{1}{2}\frac{EI}{L}(\Delta L)^2 \qquad (6)$$

where ΔL is the axial stretching deformation. The strain energy of a uniform beam under pure bending moment M is

$$u_m = \frac{1}{2}\int_0^L \frac{M^2}{EI}dL = 2\frac{EI}{L}\alpha^2 = \frac{1}{2}\frac{EI}{l}(2\alpha)^2 \qquad (7)$$

where α denotes the rotational angle at the ends of the beam. The strain energy of a uniform beam under pure torsion T is

$$u_t = \frac{1}{2}\int_0^L \frac{T^2}{GJ}dL = \frac{1}{2}\frac{T^2L}{GL} = \frac{1}{2}\frac{GJ}{L}(\Delta\beta)^2 \qquad (8)$$

where Δβ is the relative rotation between the ends of the beam and J the polar moment of inertia.

It can be concluded that U_r, U_A represent the stretching energies in the two systems (molecular and structural), U_q, U_M the bending energies, and U_ζ, U_T the torsional energies. It can be assumed that the rotation angle 2α is equivalent to the total change Δq of the bond angle, ΔL is equivalent to Δr, and Δβ is equivalent to Δϕ.

The following direct relationships between the structural mechanics parameters EA, EI and GJ and the molecular mechanics parameters k_r, k_q and k_t are obtained

$$\frac{EA}{L} = k_r; \frac{EI}{L} = k_\theta; \frac{GJ}{L} = k_r \qquad (9)$$

The above equation comprise the basis for the application of structural mechanics to the analysis of CNTs and carbon-related nanostructures. By assuming a circular beam section with diameter d, and setting

$$\mathrm{A} = \frac{\pi \mathrm{d}^2}{4}, \ \mathrm{I} = \frac{\pi \mathrm{d}^4}{64}, \ \mathrm{J} = \frac{\pi \mathrm{d}^4}{32}. \qquad (10)$$

Given the force constants k_r, k_q and k_t, the bond diameter and the elastic moduli can be obtained from eq.9

$$d = 4\sqrt{\frac{K_\theta}{K_r}} \qquad E = \frac{K_r^2 L}{4\pi k_\theta} \qquad G = \frac{K_r^2 K_\tau L}{8\pi K_\theta} \qquad (11)$$

7.2 Elastic moduli of SWCNTs:

The potential use of CNTs as reinforcing materials in nano-composites or in present advanced composites, originated the need to investigate their mechanical properties. Two of the properties receiving great attention, because they are appointing the effectiveness of CNTs, are the Young's modulus and tensile strength. Many theoretical and experimental research efforts have been placed on the investigation of Young's modulus of CNTs[5].

Young's modulus of CNTs either calculated using theoretical methods or measured using experimental techniques show a very wide scatter. The reason for that refers to the physical difficulty of direct experimental measurements, the approximable nature of theoretical methods used and mainly to the dependence of Young's modulus to various geometrical and nano-structural parameters. In the following, the FE model is applied to assess the effect of wall thickness, diameter and chirality on the Young's and shear moduli of SWCNTs.

The Young's modulus of a material is the ratio of normal stress to normal strain as obtained from a uni-axial tension test. Following this definition, the Young's modulus of SWCNTs is been calculated using the following equation

$$Y = \frac{\sigma}{E} = \frac{\frac{F}{A_o}}{\frac{\Delta H}{H_0}} \qquad (12)$$

where F is the total applied force, A_0, the cross-sectional area, H_0 the initial length and DH the elongation. A_0 is equal to $\pi\Delta t$ where D is the mean diameter of the tube. In the case of armchair and zigzag SWCNTs, their initial length H_0 is preset since, all the submarginal nodes are situated at the same plane.

However, in case of chiral SWCNTs, the submarginal nodes are not at the same plane and therefore, H_0 is taken as the average of the longitudinal coordinates of the submarginal nodes. ΔH is taken in all cases as the average of the displacements of the submarginal nodes.

For calculating the shear modulus of SWCNTs, the following relation is used

$$S = \frac{TH_o}{\theta J_\theta} \quad (13)$$

where T stands for the torque acting at the one end of the SWCNT, q for the torsional angle of the tube and J_0 for the polar moment of inertia of the cross-sectional area. For calculating J_0, the SWCNT is considered as a hollow tube of diameter D and thickness t. In this case, J_0 is equal to $(\pi/32)\{(D+t)^4-(D-t)^4\}$

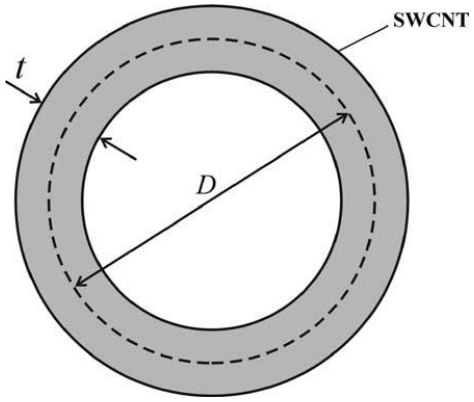


Fig. 7 DWCNT shows avg. dia[11]

The elongation ΔH and the torsional angle q are calculated by the FE model. In order to apply the conditions of tension and torsion, the nodes of the bottom end of the SWCNT have been fully bult-in (zero displacement and rotation conditions), while the nodes of the upper end, are subjected to tensile and tangential forces, respectively.

8. Vander Waals forces:

The forces of attraction which hold an individual molecule together using the covalent bonds are known as intramolecular attractions or within the layer interactions.

Vander Waals interactions are non-bonded, Intermolecular forces are attractions between one molecule and a neighboring molecule, as in our came of DWCNTs. If atoms of one layer interacts with the atom of another layer in multiwalled such interactions are due to Vander walls forces. This type of force is weak compared to covalent but one atom interacts with many atoms of the neighboring layer.

It is the distance which counts whether the force is of attractive or repulsive type and this responsiple for the stable structure model of multiwalled carbon nanotubes which maintains constant distance between the layers. As we consider the vander walls interaction also a beam elements, the number of interactions is reduced to cope with the weak, one to many interaction as in its original state.

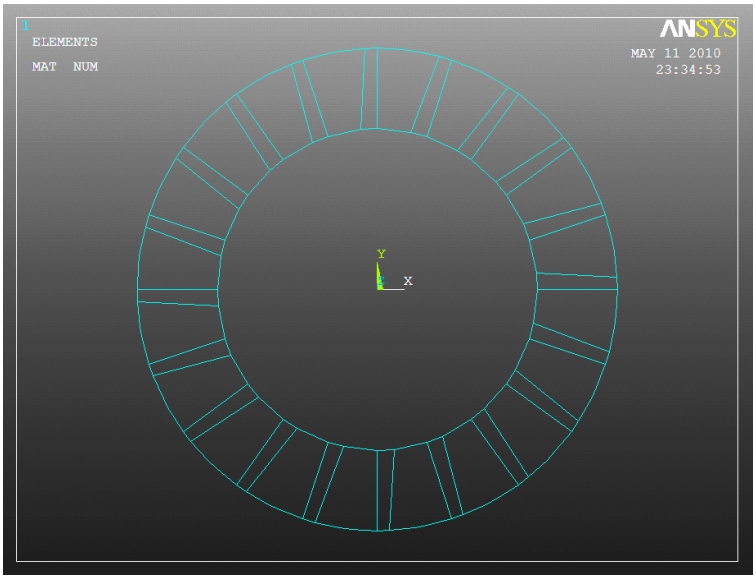


Fig. 8

The fig. 8 shows the top view of finite element mesh, the two circles denotes the two layers/walls of the carbon nanotube and lines connected between them are the Vander walls interaction, it can be observed that the two atoms were connected only with closest neighbouring layer, rest being ignored. The 10 atoms set elements is connected with 10 of the another layer and other remaining 10 being ignored.

9. Finite Element Modeling of Carbon Nanotubes using ANSYS-multiphysics:

9.1 ANSYS –FE code generated Armchair mesh:

Using the commercial code the armchair model is generated for(10,10) for 11nm length , this is the SWCNTs model i.e one layer of carbon and the beam element mesh.

Output:

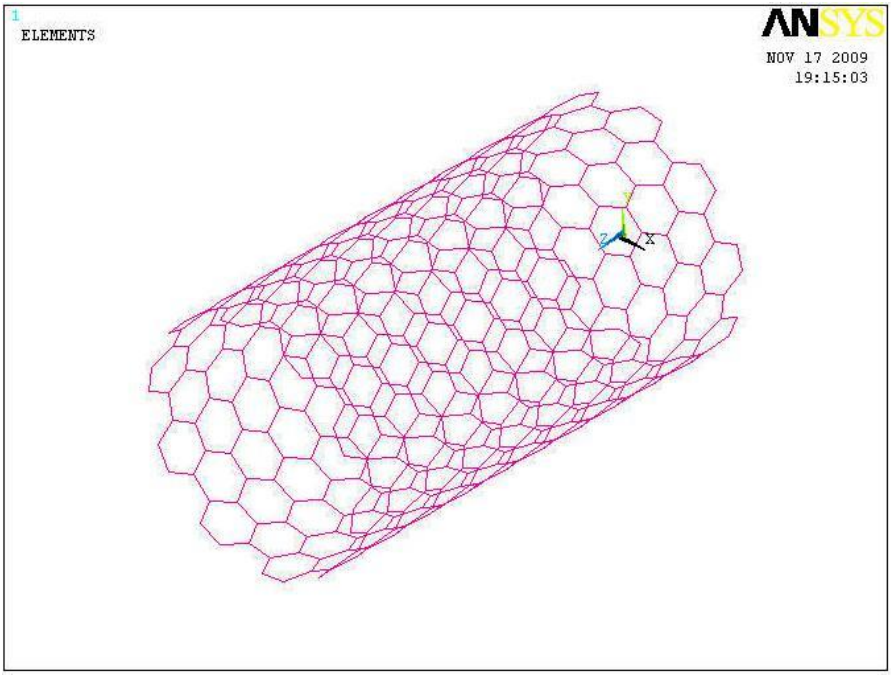


Fig. 9

The above is the mear model and no analysis is carried on as we restrict our self for multiwalled. The above model is meant to get a brief idea of single walled, beam element mesh model looks like and how one can construct the the multiwalled as above being one of the layer. Followed by few models of another type the DWCNT is also construced and analysed.

9.2 ANSYS–FE code generated for Zigzag mesh: The following shows the code generated model for Zigzag (10,0) for 11nm length, this is also of same type as armchair, the difference being the carbon atoms(node point) arrangement.

Output:

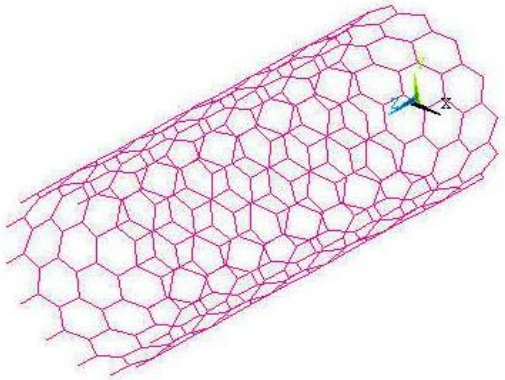
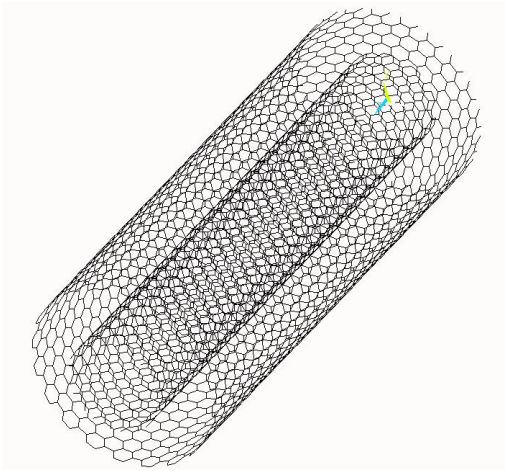


Fig. 10

9.3 ANSYS–FE code generated for DWCNT armchair mesh:

As said earlier, MWNTs are concentrically nested SWNTs, with a distance between the layers or walls equal to 0.34 nm. In DWCNT as the name suggest only two layers were considered. It is to be noted that only two layer and no vanderwall interaction is not considered here. But without the vander walls forced our model is still an incomplete one and our next step is construction of beam type interaction between molecules.



←Fig. 11 (10, 10)(20, 20) armchair ansys model, without Vander walls interaction.

10. Analysis of DWCNT:

10. 1 Static Analysis, Young modulus of DWCNT.

Static analysis is used to determine the displacements, stresses, strains, and forces in structures or componentscaused by loads that do not induce significant inertia and damping effects. Steady loading and response conditionsare assumed, that is the loads and the structure's response are assumed to vary slowly with respect to time. The kinds of load that was applied in our static analysis includes the externally applied forces. Here the nanotube which is to be analyzed should have the Vander wall interaction. By applying proper boundary conditions the analysis could be done. Here statically determinate cantilever beam is considered, so one end of the nanotube nodes all the degree of freedom is arrested. On the other end tensile forces are applied and there by the change is distance is obtained. Here the boundary conditions are applied on the node points. The youngs modulus is then obtained using the equation after solving the analysis.

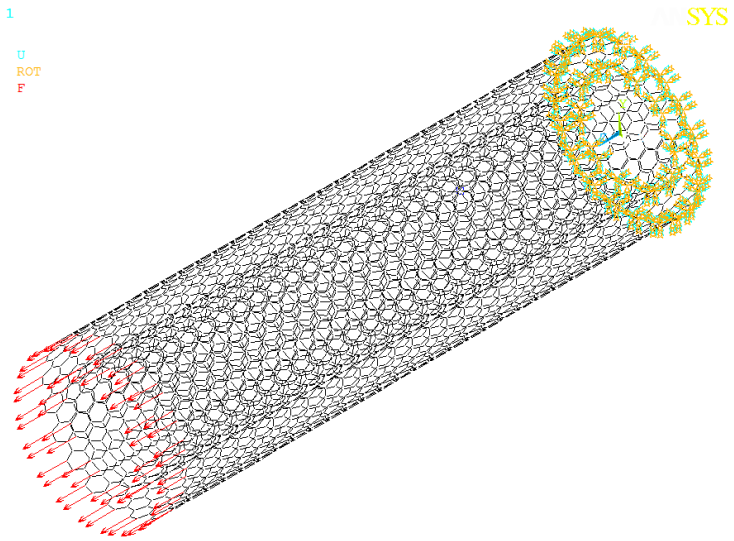


Fig. 12 DWCNT with applied boundary condition

In generalized term, build your model, apply the boundary condition, apply the load, infer the results by solving the analysis.

10.2 Modal Analysis, Vibration analysis of DWCNT:

The modal analysis is to determine the vibration characteristics namely the natural frequencies and mode shapes of a structure when it is being designed. The natural frequencies and mode shapes are important parameters in the design of a structure for dynamic loading conditions. The DWCNT was built, then as a cantilever beam the boundary conditions(supported on only one end) were applied and the solution was obtained.

11. Results and Discussion.

The following is the figure obtained after following thee previous mentioned page. This is contour obtained due to applied force of 5nN(5 nano Newton).

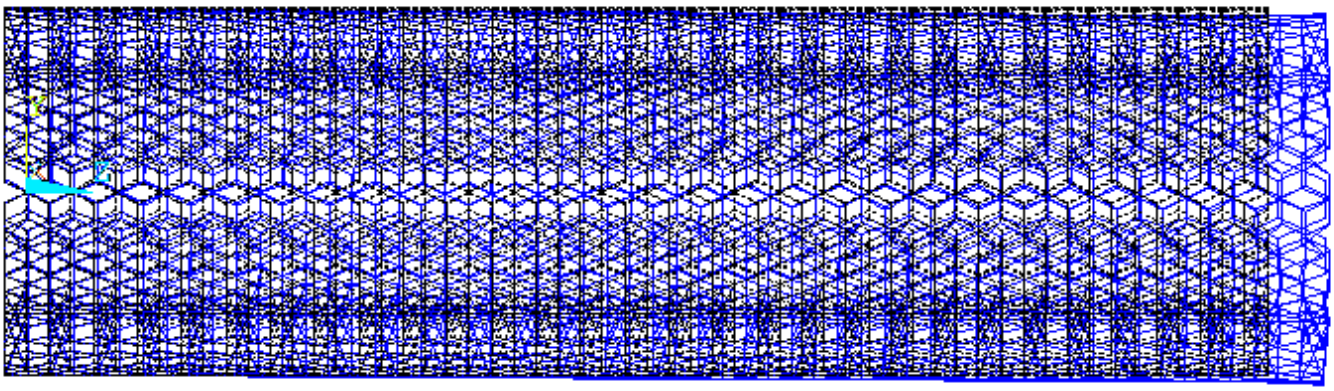


Fig. 13 The protruded out CNT is the deformation due to applied force .

The following is the table containing the properties of inner and outer layer of carbon nanotube. As explained earlier the distance between the two layers should be of 0.34 nm, hence by making the difference of two radii the exact permissible radii is obtained and it is found to be 0.34. Hence there forth our MWCNT has the credentials for the analysis as a atom like frame structure.

Table:1 Inner CNT Properties

Type	Arm-Chair
Chirality(m,n)	(10,10)
Radius	0.6784nm
No. Of Nodes	1200
No. Of Elements	1799
Length	28nm

Table:2 Outer CNT properties

Type	Armchair
Chirality(m,n)	(20,20)
Radius	1.01nm
No. Of Nodes	2457
No. Of Elements	6817
Length	28nm

By using the below equation $Y = \frac{\sigma}{E} = \frac{\frac{F}{A_o}}{\frac{\Delta H}{H_0}}$ [12], the Young's modulus is found to be **1.83TPa**.

The following take deals with the free vibrational analysis for different node

Mode	Frequency:
1	0.11250
2	0.11405
3	0.40099
4	0.49907
5	0.50141

For different mode value the corresponding frequency is obtained. One can infer from the data that the frequency increases for every mode increment, the following figures shows the different shapes of the cantilever type frame structure.

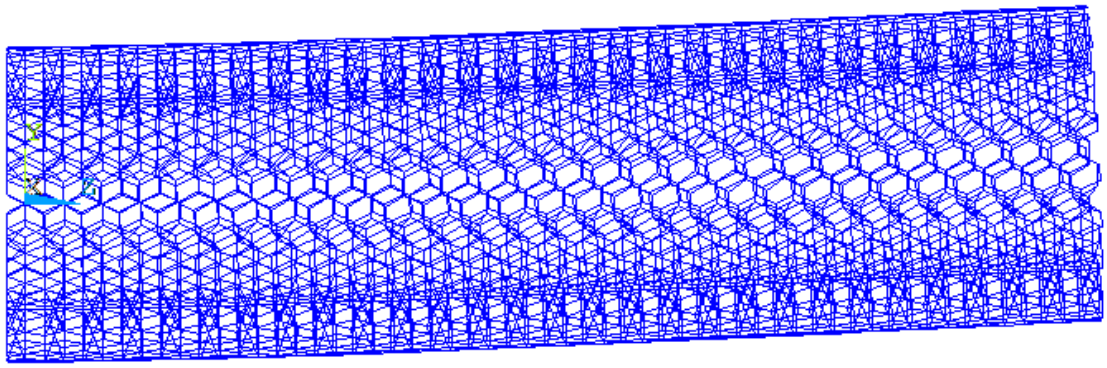


Fig. 14.a

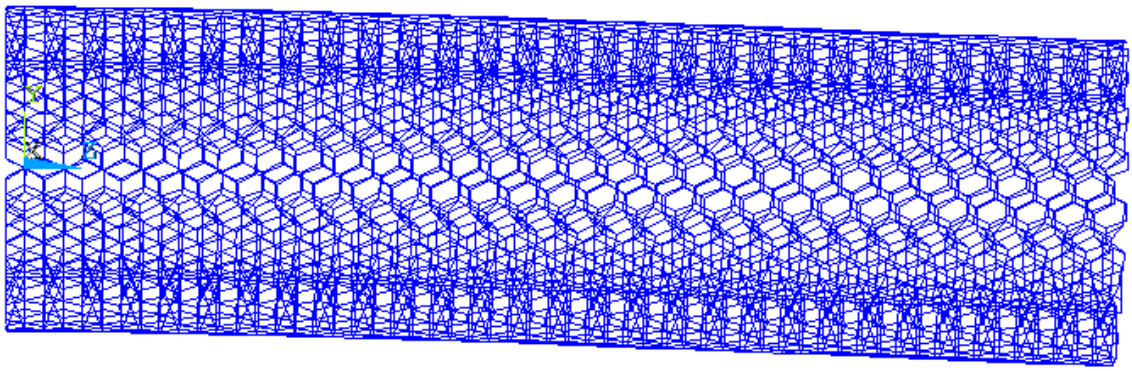


Fig. 14.b

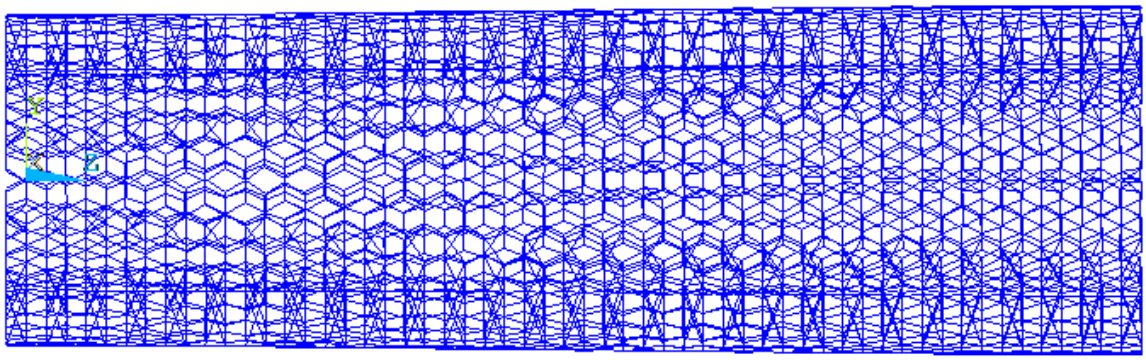


Fig. 14.c

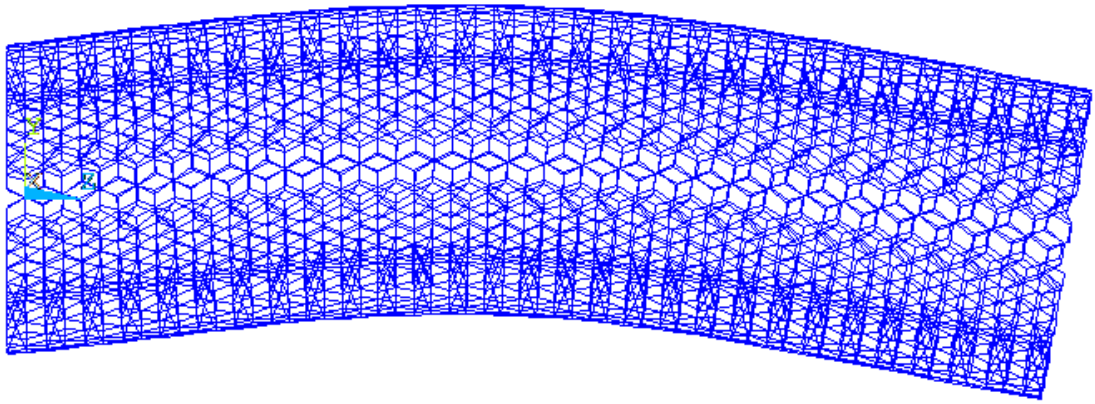


Fig. 14.d

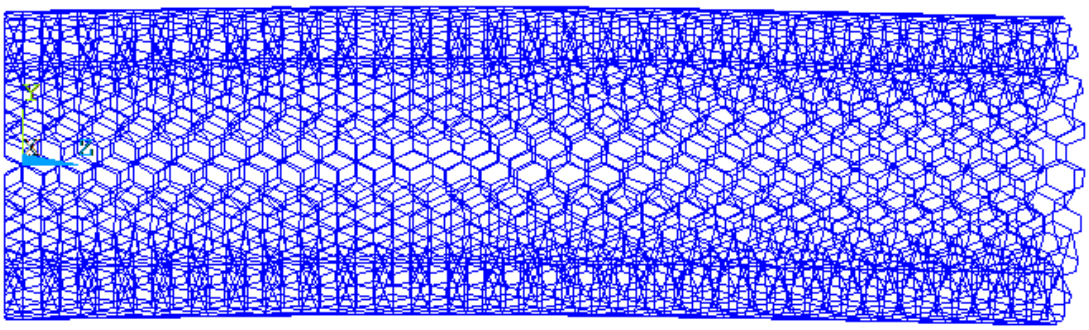


Fig. 14.e

Fig 14 a.Mode1, b.Mode2, c.Mode3, d.Mode4, e.Mode5

12. Conclusions:

The youngs modulus is found to be **1.83TPa**, were the young moduls calculated by Marino Brcic, Marko Canadija et al (FE modelling of multi-walled carbon nanotubes) was 1.04 TPa.when compared slightly same that of ours. Li and Chou obtained the Young modulus of a two layer armchair MWNT of the same diameter as Marino Brcic, Marko Canadija et al , equal to 1.05 ± 0.05 TPa. This change in our results is for a obvious reason of different radii and length. Moreover one should not forget the type of interaction we take(beam element) and the new methodology we arrived at one to one interactions. Since we arrive at close value to the above mentioned modulus by different researchers it proves our results are acceptable.

Also the frequency is also of incremented from mode1 to mode5 with respective change in the shape structure as one can easily appreciate from the figure. Hence modal analysis results are also acceptable.

Scope for future work:

For the simplification purpose the CNT the tube as such is taken, but ideally speaking the cap which surrounds the both ends of the tube should be considered. So modeling of cap and there by calculating the modulus gives the best result ever.

Also the interacting Vander wall forces the interacting is in between many to one, but we have considered one to one beam element type, few also considered one to three , so considering more gives the practical mechanical parameters.

13. Reference:

[1]**.** S. Iijima, Nature **354**, 56 (1991)

[2]. M.M.J. Treacy, T.W. Ebbesen, J.M. Gibson, Nature **381**, 678 (1996)

[3]. A. Krishmen, E. Dujardin, T.W. Ebbesen, P.N. Yianilos, M.M.J. Treacy, Phys. Rev. Lett. **58**, 14013 (1998).

[4]. E.W.Wong, P.E. Sheehan, C.M. Lieber, Science **277**, 1971 (1997)

[5]. A. Poncharal, D.M. Parks, M.C. Boyce, Science **283**, 1513 (1999)

[6]. P. Zhang, Y. Huang, H. Gao, K.C. Hwang, J. Appl. Mech. Trans. ASME **69**, 454 (2002)

[7]. P. Zhang, Y. Huang, P.H. Geubelle, P. Klein, K.C. Hwang, Int. J. Solids Struct. **39**, 3893 (2002)

[8]. C. Li, T.W. Chou, Int. J. Solids Struct. **40**, 2487 (2003)

[9]. C. Li, T.W. Chou, Compos. Sci. Technol. **63**, 1517 (2003)

[10]. C.W. Fan, J.H. Huang, C. Hwu, Y.Y. Liu, Adv. Mater. Res. **33–37**, 937 (2008)

[11]. K.I. Tserpes, P. Papanikos, Composites B **36**, 468 (2005)

[12]. Lau K-T, Hui D. The revolutionary creation of new advanced materials—carbon nanotube composites. Compos Part B Eng 2002; 33:263–77

[13]. Rappe AK, Casemit CJ, Colwell KS, Goddard WA, Skiff WM. UFF, a full periodic-table force-field for molecular mechanics and molecular dynamics simulations. J Am Chem Soc 1992;114:10024–35.

[14]. Gelin BR. Molecular modeling of polymer structures and properties. Cincinnati, OH: Hanser/Gardner Publishers; 1994.

[15]. C.W. Fan · Y.Y. Liu · Chyanbin Hwu Appl Phys A (2009) 95: 819–831DOI 10.1007/s00339-009-5080-y